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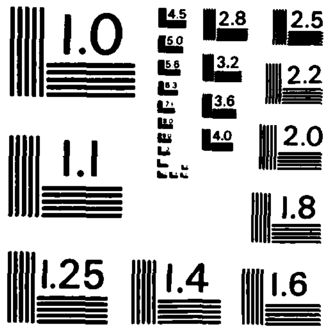

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The Lindhard, Nielsen and Scharff Method of Obtaining Approximate Cross Sections

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Scattering theory gives an exact expression for generating a differential cross section from a known interparticle potential and, conversely, if one has a cross section, there is an exact inversion process that yields the potential that is its counterpart. Lindhard, Nielsen and Scharff (LNS) developed an approximate method to generate a cross section from a potential and used this method to generate cross sections. Their Thomas-Fermi cross section is widely used in atomic scattering and radiation damage calculations.

In this report I describe the three approximations that make up the LNS method and the corresponding (approximate) inversion process. Several examples are furnished, including ones that demonstrate the utility of starting with a cross section and using the simplified inversion process to generate the corresponding approximate potential.

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CONTENTS

THE LINDHARD, NIELSEN AND SCHARFF METHOD OF OBTAINING APPROXIMATE CROSS SECTIONS

INTRODUCTION

Classical scattering theory gives an exact expression for generating a differential cross section (Go50), or, equivalently, the relation between scattering angle and impact parameter, from a known interparticle potential. Conversely, if one has an exact cross section there is an exact inversion process that yields the potential that is the counterpart of that cross section.

Lindhard, Nielsen and Scharff (LNS) developed an approximate method to generate a cross section from a potential and used this method (Li68) to generate cross sections from both power law potentials and the Thomas-Fermi potential. Their Thomas-Fermi cross section is widely used in atomic scattering and radiation damage calculations.

Given the approximations that make up the LNS method, there is an inversion procedure that generates the original potential from the approximate cross section.

In the following sections we describe the three approximations that make up the LNS method and the corresponding inversion process. We furnish several examples, including one that demonstrates the utility of starting with a cross section and using the simplified inversion process to generate the approximate potential corresponding to that cross section.

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EXACT SCATTERING RELATIONS

Consider a particle of energy E, Charge Z_1e and mass M_1 interacting with a stationary particle of charge Z_2e and mass M_2 with the interaction represented by the potential V(r). If we write the potential in the form

$$V(r) = A\ C(x) \tag{2-1}$$
$$x = r/a,$$

where a is some characteristic length, then the classical relation between the angle through which the impinging particle scatters and its impact parameter is given by (Go50)

$$\theta = \pi - 2p \int_{r_0}^{\infty} dr\ r^{-2} \left[1 - \frac{C(r/a)}{\varepsilon} - p^2 / r^2 \right]^{-1/2} , \tag{2-2}$$

where p is the impact parameter, r_0 is the distance of closest approach (the largest root of the radical in Eq. (2-2)), and ε is the dimensionless energy

$$\varepsilon = E_c / A = E\ [M_2/(M_1+M_2)] / A = E / E_L , \tag{2-3}$$

where E_c is the center of mass energy corresponding to lab energy E and the Lindhard energy unit is

$$E_L = A\ (M_1+M_2)/M_2 . \tag{2-4}$$

(For the Coulomb interaction $A=Z_1Z_2e^2/a$ and $C(x)=x^{-1}$.)

The relation between the energy T transferred in a collision and the scattering angle is

$$T = T_m \sin^2 \theta/2 , \tag{2-5}$$

where

$$T_m = \frac{4 M_1 M_2}{(M_1 + M_2)^2} E = \gamma E \tag{2-6}$$

is the maximum kinetically allowed energy transfer.

The differential cross section is given by

$$d\sigma = 2 \pi p \, dp = -2\pi \sigma_\theta \sin \theta \, d\theta = -\sigma_T \, dT . \tag{2-7}$$

LINDHARD-NIELSEN-SCHARFF SCATTERING RELATIONS

From a desire to simplify their atomic scattering and radiation damage calculations, Lindhard, Nielsen and Scharff (LNS) (Li68) made a series of approximations to the relations between the energy, impact parameter, scattering angle and cross section. They started by invoking the momentum approximation 'm', which gives the scattering angle as a function of energy and impact parameter to be (Le63)

$$\theta_m = -p/\epsilon \int_p^\infty dr \quad \frac{dC(r/a)}{dr} \; (r^2 - p^2)^{-1/2} \quad . \tag{3-1}$$

(We will use the notation of identifying letters in single quotes to indicate which approximations are being used.)

Instead of the energy transfer T they use the reduced variable

$$\eta^2 = \epsilon^2 \, T/T_m = \epsilon^2 \sin^2 \theta/2 \; . \tag{3-2}$$

They then define what they call the wide angle approximation 'w', which consists of the using the relation

$$\eta_{mw}^2 \cong \epsilon^2 \, \theta_m^2/4 \tag{3-3}$$

to replace θ, wherever it appears, by $2\eta/\epsilon$. Upon using this expression in Eq. (3-1) we obtain

$$\eta_{mw} = -\frac{1}{2}(p/a)\int_{p/a}^{\infty} dx\,[\,x^2 - (p/a)^2\,]^{-1/2}\,\frac{d}{dx}C(x) \tag{3-4}$$

Equation (3-4) provides a functional relationship between the impact parameter and the reduced energy transfer that can be used to obtain the cross section. The advantage of the LNS method is that the differential cross section depends on only one variable (either t or p/a); ordinarily there would be an explicit dependence on both p and E. LNS now write

$$d\sigma_{mw} = 2\pi\, p\, dp = 2\pi\, p(\eta)\,\frac{dp(\eta)}{d\eta}\,d\eta = -\pi\, a^2\,\eta^{-2}\,f(\eta)\,d\eta\,, \tag{3-5}$$

which defines the function $f(\eta)$ as

$$f(\eta) = -2\,\eta^2\,a^{-2}\,p(\eta)\,\frac{dp(\eta)}{d\eta} = -\eta^2\,a^{-2}\,[\,\frac{d\eta(p)}{dp^2}\,]^{-1}\,. \tag{3-6}$$

We will call $f(\eta)$ the kernel of the cross section.

The last approximation is what we might call the kinematical correction 'k', which insures that $T \to \gamma E$ as $p \to 0$. This is not the case with expression (3-4), which yields as arbitrarily large value of η as $p \to 0$. We cure this problem when evaluating Eq. (3-4) by replacing p by

$$P = [p^2 + p_0^2]^{1/2} \tag{3-7}$$

where p_0 has the value such that $\eta = \epsilon$ when $p = 0$. Thus the expression for η becomes

$$\eta_{mwk}(p) = \eta_{mw}((p^2+p_0^2)^{1/2})\,. \tag{3-8}$$

The approximation 'k' need only be invoked when explicit use is being made of the impact parameter. When working with the differential cross section as a function of η, the impact parameter does not appear.

TOTAL CROSS SECTION AND STOPPING POWER

The total cross section corresponding to expression (2-7) would be

$$2\,\pi \int_0^{\infty} dp\; p \;=\; \pi\, a^2 \int_0^{\varepsilon} d\eta\; \eta^{-2}\, f(\eta)\;, \tag{4-1}$$

but the total cross section is infinite for the infinite range potentials that we consider. One can avoid this problem by imposing a maximum allowed impact parameter or a cutoff on the energy transfer allowed at low energies.

The stopping power, which is the energy loss per unit path length, is given by

$$S(E) = 2\,\pi \int_0^{\infty} dp\; p\; T(p) \;=\; \pi\, a^2\, \frac{\gamma E_L}{\varepsilon} \int_0^{\varepsilon} d\eta\;\; f(\eta)\;. \tag{4-2}$$

The stopping power is finite, even for infinite range potentials.

We can use Eq. (3-8) to obtain relations between the impact parameter and the reduced energy transfer; within the spirit of the LNS approximations these relations are the inverses of (3-4) and (3-8). For the 'mw' case we have

$$q^2 = p^2/a^2 = \int_{\eta_q}^{\infty} d\eta\; \eta^{-2}\, f(\eta) \tag{4-3}$$

and for the 'mwk' case

$$q^2 = \int_{\eta_q}^{\varepsilon} d\eta\; \eta^{-2}\, f(\eta)\;. \tag{4-4}$$

The latter result is the more meaningful physically, but we will have need of Eq. (4-3) when we examine the inverse relations that generate potentials from approximate cross sections.

EXACT INVERSION

Just as we can calculate the scattering angle from the potential using Eq. (2-2), there is an inverse relation that yields the interaction when the scattering angle is furnished as a function of the impact parameter. Firsov (Fi53, To72) established that if we define ω as

$$\omega^2 = x^2 \left[1 - V(r)/E_c\right] \tag{5-1}$$

where E_c is the center of mass energy (Eq. (2-3)), then the interaction separation x is related to $\theta(p)$ by

$$x(\omega) = \omega \exp\left[\frac{1}{\pi} \int_\omega^\infty dp \frac{\theta(p)}{(q^2 - \omega^2)^{1/2}} \right] . \tag{5-2}$$

By using Eqs. (5-1,2) one can obtain V(r). If one uses the exact inversion procedure on an approximate cross section, the resulting interaction will be energy dependent. Robinson (Ro69) shows this effect using the LNS cross section.

IMPACT EXPANSION INVERSION

The equivalent to the Firsov procedure when one is using the momentum approximation 'm' to relate the scattering angle to the energy and impact parameter is the expression (Sm66, To72)

$$V(r) = \frac{2}{\pi} E_c \int_r^\infty dp \frac{\theta_m(p)}{(p^2 - r^2)^{1/2}} \quad . \tag{6-1}$$

In reduced form, this becomes

$$\begin{aligned} C(x) &= \frac{2}{\pi} \varepsilon \int_x^\infty dp \frac{\theta_m(q)}{(q^2 - x^2)^{1/2}} \quad , \\ &= \frac{2}{\pi} \varepsilon \int_x^\infty dp \frac{2 \sin^{-1}(\eta_m/\varepsilon)}{(q^2 - x^2)^{1/2}} \quad . \end{aligned} \tag{6-2}$$

and upon invoking the wide angle approximation we have

$$C(x) = \frac{4}{\pi} \int_x^\infty dq \; \frac{\eta_{mw}(q)}{(q^2 - x^2)^{1/2}} \; . \qquad (6\text{-}3$$

One can easily show that Eq. (3-4) and Eq. (6-3) form an inversion pair (by using Eq. (3-4) to substitute for η_{mw} in Eq. (6-3), interchanging the order of integration, and evaluating the resulting integral), as do Eq. (3-1) and Eq. (6-2). Finally, if one has the 'mwk' version of η, one uses

$$C(x) = \frac{4}{\pi} \int_x^\infty dq \; \frac{\eta_{mwk}((q^2-q_0^2)^{1/2})}{(q^2 - x^2)^{1/2}} \; . \qquad (6\text{-}4$$

One should be consistent in using these approximations when inverting to obtain a potential.

AN EXAMPLE: THE INVERSE SQUARE POTENTIAL

Let us assume an inverse square scattering potential, given by

$$V(r) = A_2 \, x^{-2} \; . \qquad (7\text{-}1$$

Eq. (2-2) yields the exact scattering angle and reduced energy transfer

$$\theta = \pi \, [1 - q(q^2 + 1/\epsilon)^{-1/2}] \qquad (7\text{-}2$$
$$\eta = \epsilon \cos \pi q/(2(q^2+1/\epsilon)) \; .$$

In the momentum approximation the energy transfer becomes

$$\eta_m = \epsilon \sin \pi/(4\epsilon q^2) \; . \qquad (7\text{-}3$$

With the the use of the wide angle and kinematic approximations the reduced energy transfer becomes

$$\eta_{mw} = \pi/(4q^2) \; , \qquad (7\text{-}4$$

and

$$\eta_{mwk} = \epsilon / (1+4\epsilon q^2/\pi) \ , \tag{7-5}$$

respectively.

We can compare the various approximations for the inverse square potential by evaluating the exact potential that corresponds to each of the approximate energy transfer relations, that is, to each approximate cross section. We use the exact inversion in the form of Eq. (5-1) and

$$x(\omega) = \omega \exp[\ \frac{1}{\pi} \int_{\omega}^{\infty} dq\ \frac{2 \sin^{-1}(\eta/\epsilon)}{(q^2 - \omega^2)^{1/2}}\ ] \ . \tag{7-6}$$

Of course, if we use the exact expression (7-2) we obtain $C(x)=x^{-2}$. For the others, we can make expansions in $1/x^2$, thus obtaining the results in the form

$$C(x) = \sum_{m=0} b_m\ \epsilon^{-m}\ x^{-2m-2} \ . \tag{7-7}$$

The first few coefficients b_m for the three approximations are given in Table 1.

Table 1

Coefficient b_m of $\epsilon^{-m}\ x^{-2m-2}$ in Eq. (7-7)

Index	Exact Value	Approximation 'm'	Approximation 'mw'	Approximation 'mwk'
0	1	1	1	1
1	0	.50000	.50000	-.02360
2	0	.66667	.72150	.00329
3	0	1.12500	1.28949	-.00071
4	0	2.13333	2.58358	.00019

We see that the combined 'mwk' approximation gives a cross section whose corresponding potential more closely agrees with the exact cross section than do the other approximations. In this regard we should mention that for the Coulomb potential, the 'mwk' approximation is identical to the exact cross section.

AN EXAMPLE: THE POWER LAW KERNEL

There are cases in which we start with a cross section directly, rather than calculating one from a potential. Consider the kernel

$$f_n(\eta) = B\ \eta^{1-2/n} \ . \qquad \text{(8-1}$$

By using the relation (4-3) we have

$$q^2 = \int_\eta^\infty ds\ s^{-2}\ B\ s^{1-2/n} = \frac{n}{2} B\ \eta^{-2/n} \qquad \text{(8-2}$$

or

$$\eta = \left[\frac{n\ B}{2\ q^2}\right]^{n/2} \qquad \text{(8-3}$$

as the relation between the impact parameter and reduced energy transfer. Upon using the inversion formula (6-3) we find

$$C_n(x) = \frac{4}{\pi} \left(\frac{n\ B}{2}\right)^{n/2}\ x^{-n} \int_0^{\pi/2} d\beta\ \sin^{n-1}\beta \qquad \text{(8-4}$$

The various constants, including the integral, don't interest us, but we see that our kernel is equivalent to a power law x^{-n} potential. We note that for the Coulomb potential, for which $C_1(x)=x^{-1}$, B will have the value $B=1/2$ and $f_1(\eta)=1/(2\eta)$.

The point of this exercise is to illustrate that we can start with some simple form for the cross section and use the inversion relations to determine the equivalent potential, within the LNS approximations.

AN EXAMPLE: A SIMPLE KERNEL FOR A FINITE RANGE POTENTIAL

Assume the kernel

$$f(\eta) = (1/2)\ \eta^2/(\beta+\eta)^3\ . \qquad (9\text{-}1$$

We see that for large values of η, corresponding to high momentum transfers, this $f(\eta)$ tends toward the Coulomb kernel. By using the relation (4-3) we have

$$q^2 = (1/4)\ (\beta+\eta)^{-2} \qquad (9\text{-}2$$

or

$$\eta = 1/2q - \beta \qquad (9\text{-}3$$

as the relation between the impact parameter and reduced energy transfer. We see that zero energy transfer (η=0) corresponds to a maximum value of the impact parameter of

$$x_m = 1/(2\beta)\ . \qquad (9\text{-}4$$

Upon using the inversion formula (6-3) we find

$$C(x) = x^{-1}\ [2/\pi]\ [\cos^{-1} y\ -\ y\ \ln((1+(1-y^2)^{1/2})/y)] \qquad (9\text{-}5$$

where

$$y=x/x_m\ . \qquad (9\text{-}6$$

Note that upon setting β to zero (y=0) one recovers the reduced Coulomb potential $C(x)=1/x$. The quantities in square brackets in Eq. (9-5) constitute the finite range screening factor for the Coulomb interaction.

In Fig. 1 we illustrate the effect of this screening factor. Rather than set β to different values directly, we will choose various values of $x_m=1/(2\beta)$. For atomic scattering problems a typical screening radius

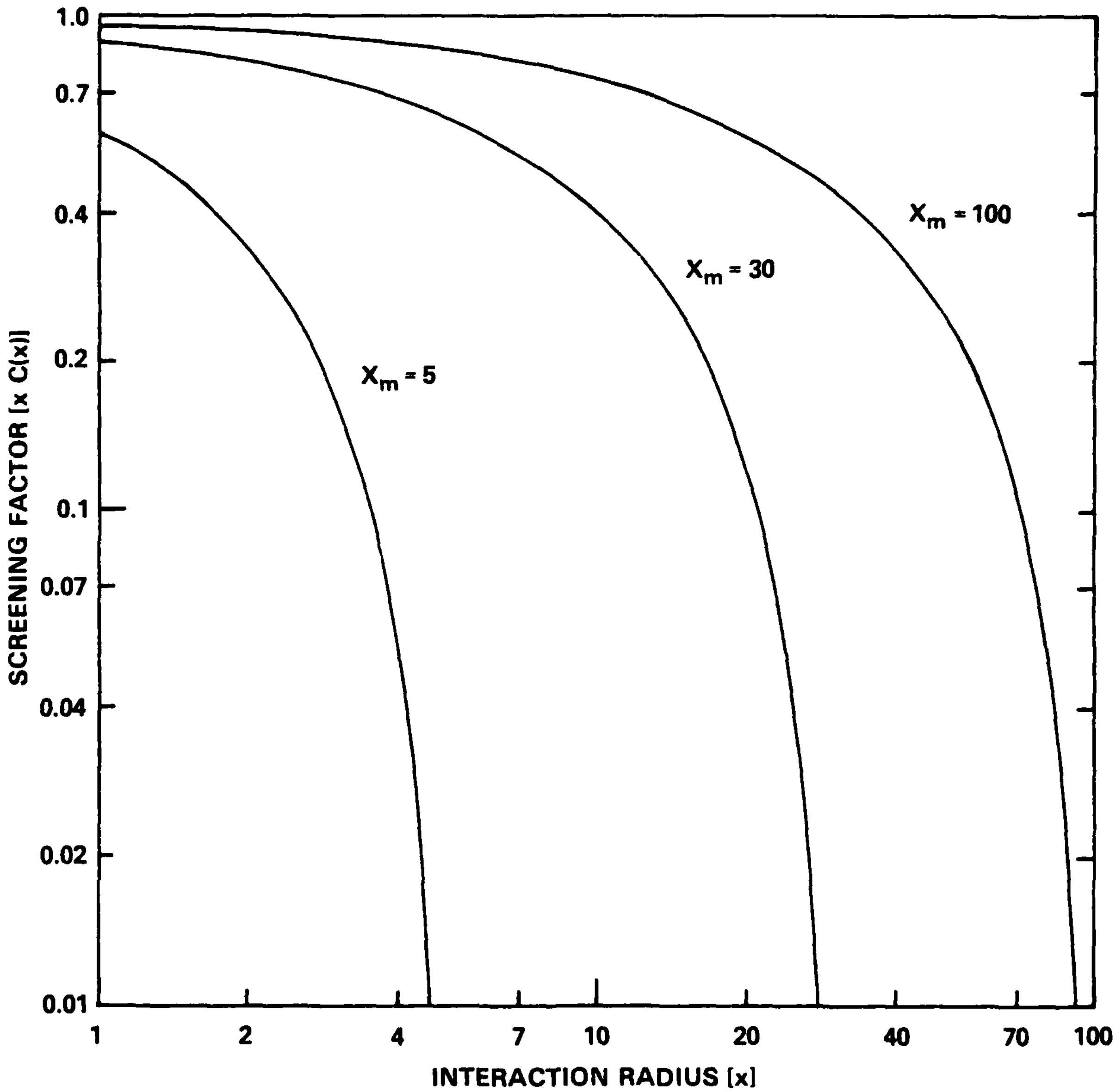

Fig. 1: The interactomic screening factor corresponding to the kernel $f(\eta) = (1/2)\ \eta^2/(\beta+\eta)^3$ for three values of $x_m = 1/(2\beta)$.

(Eq. (2-1)) is a=0.01 nm, so that x_m=100 corresponds to a cutoff radius of 1.0 nm. Figure 1 shows the screening factor for three potentials derived from the cross section (9-1), using values of x_m= 5, 30, and 100.

If one had a simple, finite range, phenomenological potential with Coulomb behavior at small separations, one could fit that potential by adjusting β (or x_m), obtaining in the process a simple cross section corresponding to that potential. This same procedure can be used to fit a wide variety of phenomenological potentials with forms whose corresponding cross sections are simple (Mu85).

NUMERICAL EVALUATION

When using numerical methods to evaluate the inversion integrals, it is advantageous to modify formula (6-3) by a change of variable (from q to η) and an integration by parts. This yields

$$C(x) = \frac{4}{\pi} \int_0^{\eta_x} d\eta \ (q^2 - x^2)^{1/2} \left[\frac{1}{q} - \frac{\eta q'}{q^2}\right] \qquad (10\text{-}1$$

where q and q' are functions of η. The variable η_x is implicitly given by

$$x^2 = \int_{\eta_x}^{\infty} d\eta \ \eta^{-2} f(\eta) \ . \qquad (10\text{-}2$$

and the function $q(\eta)$ is

$$q^2 = \int_{\eta}^{\infty} ds \ s^{-2} f(s) \ ; \qquad (10\text{-}3$$

q' is simply

$$q' = -\eta^{-2} f(\eta) \ / \ (2q) \qquad (10\text{-}4$$

so that

$$C(x) = \frac{4}{\pi} \int_0^{\eta_x} d\eta \; (q^2 - x^2)^{1/2} \; [\frac{1}{q} + \frac{f(\eta)}{2\eta q^3}] \qquad (10\text{-}5$$

The inversion proceoure consists of:

a) Choosing some value for η_x and using Eq. (10-2) to determine the corresponding value of x.

b) Choosing a set of integration points for the numerical integration of Eq. (10-5) and using Eq. (10-3) to determine the corresponding value of q.

Often, if the kernel $f(\eta)$ is some simple form, then the integral (10-3) can be done exactly. If Eq. (10-3) must be evaluated numerically, then one can use the form

$$q^2 = x^2 + \int_{\eta}^{\eta_x} d\eta \; \eta^{-2} f(\eta) \; . \qquad (10\text{-}6$$

DISCUSSION

To extend the discussion of the last two sections, many radiation damage calculations, such as Boltzmann transport theory calculations, use a cross section directly without any reference to the potential. For such numerical work a simple cross section can save computer time.

Our earlier treatment of the Moliere potential serves as an example. The Moliere is an approximation to the Thomas-Fermi interaction that has an exponential tail instead of the Thomas-Fermi's x^{-4} dependence at large separations (Mo49, To72a, Ro69).

In order to generate a useful cross section we (Mu78, Mu80):

a) Used the LNS procedure to generate the kernel $f_M(\eta)$ corresponding to the Moliere potential.

b) Created an approximate fit to $f_M(\eta)$ that was expeditious for machine calculations.

c) Used the approximate inversion procedure to examine the aeviation (within the LNS approximations) of the potential corresponding to our fit and the Moliere potential.

This method allowed us to find a simple form for the cross section that reproduced the Moliere potential to within six per cent.

The simplicity of the LNS inversion pairs generally makes it easy to create a usable fit to the cross section corresponding to a given atom–atom interaction.

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